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Modeling structure property relationships using finite elements and high energy X-rays

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ABSTRACT

Mechanical design with structural materials has been well-served by traditional methods for linking microstructure to mechanical properties using image-based data and mechanical testing. Modern “micrographs” might include three-dimensional microstructural models with spatially resolved orientation and/or chemical composition. Regardless of the level of detail, however, image-based data contain no information regarding the mechanical response of the aggregate. Often the connections between the microstructure and resulting mechanical properties are derived by intuition and inference. This highly empirical process is one of the reasons that materials design and selection are such time and resource-intensive process. The creation of mathematical models of the microstructure – ones based on functional accuracy – was the motivation of the Integrated Computational Materials Engineering report and the Materials Genome Initiative. Once deemed “reliable” such models could be employed to conduct costly “microstructural iterations” to optimize properties. This discussion describes a method for studying structure–property relations using a finite element representation of the crystal and subcrystal scale microstructure. A key aspect of the methodology is a set of high energy X-ray diffraction experiments with in situ mechanical loading and heating designed to provide crystal-scale micromechanical material response data. Bringing the experimental and simulated data into coincidence builds trust in the model and its ability to enable optimizations during the material design process. Examples employing various experimental methods and functional material representations are described examining a range of engineering materials.